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Energy levels, oscillator strengths and lifetimes in Cl VI

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Abstract We have calculated energy levels, oscillator strengths and transition probabilities for all dipole-allowed transitions among the 24 terms belonging to the $(1s^2 2s^2 2p^6)3s^2$, $3s3p$, $3p^2$, $3s3d$, $3s4s$, $3p3d$ $3s4p$, $3s4d$, $3s4f$ and $3p4s$ configurations of Cl VI in the LS coupling scheme. We included fairly large number of configurations in the configuration-interaction expansions to ensure convergence. The calculated energy levels are in close agreement with laboratory measurements. From our transition probabilities, we have also calculated radiative lifetimes of 12 singlet and 10 triplet states in Cl VI. The present results are compared with the other available theoretical results.

Keywords Atomic energy levels, oscillator strength, transiton probability

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1. Introduction

Elements in the Mg isoelectronic sequence are astrophysically abundant and accurate atomic data such as absorption oscillator strengths, and transition probabilities are needed for the interpretation of accurate observational data. These atomic data are also useful in many astrophysical studies.

Most of the results available in the literature for the ions of Mg isoelectronic sequence are limited to allowed transitions involving the few lowest states [1- 16]. The study of Mg-like sulphur and chlorine are of particular interest [16]. For Mg-like chlorine, only few calculations are available in LS coupling scheme [2,7,9]. Victor *et al* [2] performed a configuration-interaction (CI) calculation of oscillator strengths in the Mg isoelectronic sequence (including S V and Cl VI) within a semiempirical model potential framework. Froese Fischer and Godefroid [7] calculated the lifetimes for all bound singlet states in the $n = 3$ complex of the Mg sequence for $Z \leq 26$ using multi-configuration Hartree-Fock (MCHF) wavefunctions. Godefroid and Froese Fischer [9] reported the oscillator strengths and transition probabilities for S V and Cl VI in MCHF and multi-configuration Hartree-Fock with Breit-Pauli corrections (MCHF-BP) methods.

Recently, Gupta and Msezane [11] calculated energy levels, oscillator strengths, and transition probabilities for all dipole-allowed transitions among the 24 LS target states $3s^2(^1S)$, $3s3p(^{1,3}P^0)$, $3p^2(^1S, ^3P, ^1D)$, $3s3d(^{1,3}D)$, $3s4s(^{1,3}S)$, $3p3d(^{1,3}P^0, ^{1,3}D^0, ^{1,3}F^0)$, $3s4p(^{1,3}P^0)$, $3s4d(^{1,3}D)$, $3s4f(^{1,3}F^0)$ and $3p4s(^{1,3}P^0)$ of Mg-like sulphur in LS coupling scheme using the CIV3 computer code of Hibbert [17]. In the present work, we have extended our calculation of these parameters for Mg-like chlorine. From our transition probabilities, we have also calculated radiative lifetimes of singlet and triplet states in Cl VI.

2. Choice of radial functions and configurations

In our calculation, we used the 15 orthogonal one-electron orbitals . $1s$, $2s$, $2p$, $3s$, $3p$, $3d$, $4s$, $4p$, $4d$, $4f$, $5s$, $5p$, $5d$, $5f$ and $5g$. The $1s$, $2s$ $2p$ and $3s$ radial functions are chosen as the Hartree-Fock (HF) functions of the ground state $(1s^2 2s^2 2p^6)3s^2(^1S)$ of Cl VI given by Clementi and Roetti [18] and the remaining radial functions have been obtained

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using CIV3 computer code of Hibbert [17]. The ionic state wave functions are written in terms of CI expansions

$$\Psi(LS\pi) = \sum_{i=1}^{M} a_i \phi_i(\alpha_i LS\pi), \quad (1)$$

where each single-configuration function ϕ_i is constructed from one-electron orbitals whose angular momenta are coupled to give total L, S and π. M is the number of configurations and α_i specify the angular momentum coupling scheme of the i-th configuration. The radial parts of the one-electron functions are expressed in analytic form as a sum of Slater-type orbitals

$$P_{nl} = \sum_{i=1}^{k} C_i \left[(2\xi_i)^{2p_i+1}/(2p_i)!\right]^{1/2} r^{p_i} \exp(-\xi_i r) \quad (2)$$

The parameters C_i, ξ_i and p_i in eq. (2) are determined variationally as described by Hibbert [17].

The $3p$, $3d$, $4s$, $4p$, $4d$ and $4f$ functions are chosen as spectroscopic-type and are optimized on the excited states $3s3p(^3P^0)$, $3s3d(^3D)$, $3s4s(^3S)$, $3s4p(^3P^0)$, $3s4d(^3D)$, and $3s4f(^3F^0)$ respectively. There is a strong mixing between the $3p3d(^1P^0)$ and $3s4p(^1P^0)$ levels because of their proximity. We have chosen the $5s$, $5p$, $5d$, $5f$, and $5g$ functions as correlation-type and optimized them on the $3d4d(^1D)$, $3p3d(^3D^0)$, $3p3d(^1F^0)$, $3p3d(^3D^0)$, and $3s3d(^1F^0)$ states, respectively. It is necessary to use the correlation functions in addition to the spectroscopic functions so that a single set of orthogonal functions can represent all the energy levels. In all cases, we chose $k = n - 1$ so that the coefficients C_i are uniquely specified by the orthogonality condition on P_{nl} [17].

In order to test the convergence of CI expansions for different LS symmetries, we carried out several test calculations. In our largest calculation, we considered up to two-electron excitation from the basic configurations used in this calculation. All configurations with weight more than 0.005 are retained in our final calculation. We considered configurations within the $n = 5$ complex in the CI expansion to ensure convergence. The CI wave functions, in eq. (1), are used to calculate energy levels, oscillator strengths, and radiative transition probabilities.

The absorption oscillator strengths in length and velocity form are calculated using the relations [19]

$$f_{ij}^{L} = [2\Delta E/3]\left|\langle \psi_j | r | \psi_i \rangle\right|^2, \quad (3)$$

$$f_{ij}^{V} = [2/3\Delta E]\left|\langle \psi_j | \nabla | \psi_i \rangle\right|^2, \quad (4)$$

and the radiative lifetime of an excited state is obtained from radiative transition probabilities A_{ji} as

$$\tau_j = 1/\Sigma_i A_{ji}, \quad (5)$$

where the sum over i is over all accessible final states. ΔE ($= E_j - E_i$), is the transition energy.

3. Results and discussion

3.1 Energy levels

In Table 1, we present our *ab initio* calculation of excitation energies of the 24 low-lying levels relative to the ground level. These are compared with the experimental results of Jupen and Fremberg [20]. It is seen from the table that the ordering of our calculated excitation energies is the same as that of the experiment data. Our energy values agree to better than 1% with the measured values, except for the $3s4d(^3,^1D)$ and $3s4f(^3,^1F^0)$ states where the experimental data is missing.

Table 1. Calculated and experimental energy levels (in a.u.) of Cl VI

Index	Level		Present	Experiment*
1	$3s^2$	^1S	0.0000	0.0000
2	$3s3p$	$^3P^0$	0.4426	0.4521
3		$^1P^0$	0.6814	0.6787
4	$3p^2$	^1D	1.0299	1.0444
5		^3P	1.0673	1.0759
6	$3s3d$	^3D	1.2641	1.2749
7	$3p^2$	^1S	1.2563	1.2575
8	$3s3d$	^1D	1.4622	1.4623
9	$3s4s$	^3S	1.8431	1.8559
10		^1S	1.8921	1.9016
11	$3p3d$	$^3F^0$	1.7313	1.7519
12		$^1D^0$	1.7568	1.7746
13		$^3P^0$	1.8507	1.8636
14		$^3D^0$	1.8644	1.8774
15	$3s4p$	$^3P^0$	2.0494	2.0647
16		$^1P^0$	2.0780	2.0858
17	$3p3d$	$^1F^0$	1.9870	1.9966
18		$^1P^0$	2.0144	2.0207
19	$3s4d$	^3D	2.3078	
20		^1D	2.3134	
21	$3s4f$	$^3F^0$	2.3960	
22		$^1F^0$	2.4309	
23	$3p4s$	$^3P^0$	2.4242	2.4407
24		$^1P^0$	2.4596	2.4638

*Jupen and Fremberg [20]

3.2 Oscillator strengths and radiative decay rates

In Table 2, our radiative decay rates in the length approximation A_l and the absorption oscillator strengths in both length f_l and velocity f_v formulations, for all dipole-allowed transitions among the 24 LS levels are listed. There is very good agreement between length and velocity values of oscillator strengths for most transitions, to some extent, indicating the overall good accuracy of our wave functions used in calculating these parameters. Our results are compared with the theoretical values of Froese Fischer and Godefroid [7], Godefroid and Froese Fiscer [9], and Victor *et al* [2]. All calculations agree well for almost all the strong transitions

Table 2. Transition probabilities and oscillator strengths for allowed transitions in Cl VI

Transitions	Present calculation			Other calculations			
				FFG			VSL
	A_L	f_L	f_l	A_l	f_l	f_l	
$3s^2(^1S)$–$3s3p(^1P^0)$	6 6324+09	1 3336	1 3756	6 500+09	1 320	1 330	1 2700
$3s4p(^1P^0)$	3 9292+09	0 0850	0 0807				0 0916
$3p3d(^1P^0)$	2 2201+09	0 0511	0 0518	1 720+09	0 039	0 038	0 0934
$3p4s(^1P^0)$	2 6305+06	0 0000	0 0000				0 0023
$3s3p(^1P^0)$–$3p^2(^1D)$	2 7056+08	0 1156	0 1114	2 750+08	0 119	0 110	0 1160
$3p^2(^1S)$	5 4704+09	0 1717	0 1840	5 330+09	0 173	0 179	0 1650
$3s3d(^1D)$	1 5038+10	1 2796	1 3374	1 497+10	1 273	1 323	1 2400
$3s4s(^1S)$	1 1260+10	0 0797	0 0802				0 0691
$3s4d(^1D)$	1 7572+09	0 0342	0 0264				0 0252
$3p^2(^1D)$–$3p3d(^1D^0)$	6 4773+09	0 3816	0 4049	6 430+09	0 378	0 396	0 3620
$3s4p(^1P^0)$	1 4894+09	0 0253	0 0264				0 0219
$3p3d(^1F^0)$	1 2183+10	0 5795	0 6011	1 252+10	0 594	0 626	
$3p3d(^1P^0)$	1 5985+09	0 0308	0 0316	8 920+08	0 0168	0 0134	0 0377
$3s4f(^1F^0)$	3 0924+09	0 0686	0 0668				
$3p4s(^1P^0)$	1 1954+10	0 1092	0 1112				0 1080
$3p^2(^1S)$–$3s4p(^1P^0)$	3 8587+09	0 5335	0 5554				0 6570
$3p3d(^1P^0)$	5 5991+09	0 9097	0 9675	7 100+09	1 120	1 210	0 6640
$3p4s(^1P^0)$	2 2456+09	0 1448	0 1567				0 1200
$3s3d(^1D)$–$3p3d(^1D^0)$	9 9928+07	0 0358	0 0331	1 010+08	0 0366	0 0334	0 0344
$3s4p(^1P^0)$	1 0184+08	0 0050	0 0060				0 0111
$3p3d(^1F^0)$	3 1240+09	0 4942	0 5223	3 020+09	0 482	0 488	
$3p3d(^1P^0)$	3 6433+09	0 2232	0 2394	4 070+09	0 244	0 266	0 2150
$3s4f(^1F^0)$	2 1214+10	0 9850	0 9868				
$3p4s(^1P^0)$	3 2987+09	0 0619	0 0624				0 0464
$3s3s(^1S)$–$3s4p(^1P^0)$	1 5586+08	0 4208	0 5298				0 3910
$3p3d(^1P^0)$	2 6520+07	0 1656	0 1881				0 2400
$3p4s(^1P^0)$	3 3455+09	0 9697	1 0066				1 0400
$3p3d(^1D^0)$–$3s4d(^1D)$	1 1573+07	0 0012	0 0014				0 0014
$3s4p(^1P^0)$–$3s4d(^1D)$	4 7357+08	0 4433	0 4403				0 3770
$3p3d(^1F^0)$–$3s4d(^1D)$	1 5887+08	0 0331	0 0244				
$3p3d(^1P^0)$–$3s4d(^1D)$	6 0203+08	0 3491	0 3209				0 4120
$3s4d(^1D)$–$3s4f(^1F^0)$	9 2454+07	0 2917	0 2312				
$3s4d(^1D)$–$3p4s(^1P^0)$	2 2321+05	0 0002	0 0082				0 0034
$3s3p(^1P^0)$–$3p^2(^1P)$	5 6745+09	0 4526	0 4713				0 4300
$3s3d(^3D)$	8 4198+09	0 6472	0 6779				0 6120
$3s4s(^3S)$	1 8159+10	0 0961	0 0986				0 0941
$3s4d(^3D)$	4 4049+09	0 0657	0 0649				0 0717
$3p^2(^3P)$–$3p3d(^3P^0)$	6 7401+09	0 3418	0 3630				0 3240
$3p3d(^3D^0)$	1 1925+10	0 9736	1 0337				0 9240
$3s4p(^3P^0)$	2 4590+06	0 0001	0 0002				0 0000
$3p4s(^3P^0)$	1 0856+10	0 1835	0 1867				0 1720
$3s3d(^1D)$–$3p3d(^1F^0)$	1 0368+09	0 2070	0 2095				
$3p3d(^1P^0)$	2 8060+09	0 1523	0 1616				0 1450
$3p3d(^3D^0)$	2 6547+09	0.2293	0 2421				0 2180
$3s4p(^3P^0)$	3 0024+09	0 0909	0.0937	2 951+09*	0 091*		0 1000
$3s4f(^3F^0)$	2 5925+10	0.8817	0.8821				
$3p4s(^3P^0)$	9 9343+07	0 0014	0 0017				0 0014

Table 2. *(Cont'd.)*

Transitions	Present calculation			Other calculations		
				FFG		VSL
	A_l	f_l	f_v		f_l	
$3s4s(^3S)$ $3p3d(^1P^0)$	3 8348+00	0 0000	0.0000			0 0000
$3s4p(^3P^0)$	4 1177+08	0 9032	0 9220	4 124+08*	0 898*	0 9200
$3p4s(^1P^0)$	2 7012+09	0 7470	0 7820			0 7040
$3p3d(^3F^0)$–$3s4d(^3D)$	1 5018+08	0 0100	0 0094			
$3p3d(^1P^0)$–$3s4d(^1D)$	7 5650+05	0 0002	0 0001			
$3p3d(^1D^0)$–$3s4d(^1D)$	5 1511+05	0 0001	0 0002			0 0012
$3s4p(^3P^0)$–$3s4d(^3D)$	1 0522+09	0 8175	0 7759			0 7940
$3s4d(^1D)$–$3s4f(^1F^0)$	4 0335+07	0 2259	0 1982			
$3s4d(^1D)$–$3p4s(^3P^0)$	7 0092+05	0 0010	0 0030			0 0007

VSL Calculation of Victor *et al* [2], FFG Calculation of Froese Fischer and Godefroid [7], * Results of Godefroid and Froese Fischer [9]

except those involving $3p3d(^1P^0)$ and $3s4p(^1P^0)$ levels. As we pointed out earlier, there is a strong mixing between these two levels. In our CI calculation, the eigenvector composition for these two states are as follows :

$$3s4p(^1P^0) = 0.768\ 3s4p(^1P^0) + 0.593\ 3p3d(^1P^0),$$

$$3p3d(^1P^0) = 0.573\ 3s4p(^1P^0) + 0.778\ 3p3d(^1P^0).$$

The small oscillator strengths are sensitive to cancellation effects and for weaker transitions, we find a significant difference between our results and the calculation of Victor *et al* [2].

3.3 *Lifetimes*

In Table 3, we present our calculated radiative lifetimes (using eq. (5)) for singlet and triplet states. The results of Froese Fischer and Godefroid [7] are also included for the comparison. There is an excellent agreement between the two calculations.

Table 3. Lifetimes (in nanoseconds) of singlet and triplet states in Cl VI

Upper State	Present	FFG*
$3s3p(^1P^0)$	0 1508	0 15
$3p^2(^1D)$	3 6960	3 6
$3p^2(^1S)$	0 1828	0 190
$3s3d(^1D)$	0 0665	0 067
$3s4s(^1S)$	0 0888	
$3p3d(^1D^0)$	0.1520	0 15
$3s4p(^1P^0)$	0.1049	
$3p3d(^1F^0)$	0 0653	0 064
$3p3d(^1P^0)$	0 0764	0 073
$3s4d(^1D)$	0 3330	
$3s4f(^1F^0)$	0 0410	
$3p4s(^1P^0)$	0 0480	
$3p^2(^1P)$	0.1762	
$3s3d(^3D)$	0 1188	

Table 3. *(Cont'd)*

Upper State	Present	FFG*
$3s4s(^3S)$	0 0551	
$3p3d(^3F^0)$	0 9645	
$3p3d(^3P^0)$	0 1048	
$3p3d(^3D^0)$	0 0686	
$3s4p(^3P^0)$	0 2927	
$3s4d(^3D)$	0 1783	
$3s4f(^3F^0)$	0 0385	
$3p4s(^3P^0)$	0 0759	

*Calculation of Froese Fischer and Godefroid [7]

4. Conclusion

In conclusion, we have presented an extensive CI calculation of energy levels, oscillator strengths and transition probabilities for all dipole-allowed transitions among the 24 terms arising from the terms belonging to the $(1s^22s^22p^6)3s^2$, $3s3p$, $3s3d$, $3p^2$, $3p3d$, $3s4s$, $3s4p$, $3s4d$, $3s4f$ and $3p4s$ configurations of Cl VI. Our *ab initio* energies presented in this paper, are in excellent agreement with the measurement of Jupen and Fremberg [20] for all the excited states. Also a very good agreement between the length and velocity values of our oscillator strengths for most transitions, is indicative of the overall accuracy of wave functions used in this calculation. Generally, our results agree reasonably well with the available theoretical calculations. Finally, our results are more extensive and we believe that they would be useful in many astrophysical applications.

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